A Parallel, 3D Baroclinic Shallow Water Model

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LONG-TERM GOALS

The long-term goal of this research is to develop an efficient, robust hydrodynamic model that is capable of three-dimensional (3D), prognostic baroclinic simulations on a parallel computing platform. Our approach is to modify an existing model ADCIRC (ADvanced 3D CIRCulation model [1]), which is the product of over 20 years of research and development by scientists and engineers at six different institutions. Among other military and civilian applications, ADCIRC is currently one of a suite of models used by the Office of Naval Research's (ONR) Naval Research Lab (NRL) at Stennis Space Center, MS, to help plan Naval fleet operations in ocean basins around the world. The improved ADCIRC model would further enhance NRL's ability to provide accurate, timely nowcasts/forecasts, particularly in thermohaline driven basins, like the Persian Gulf (see Figure 1).

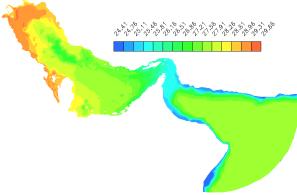


Figure 1. Diagnostic density field (bottom layer) for the Persian Gulf. Note that the large density gradients produce a large baroclinic pressure gradient field that can result in currents that equal or exceed those generated by the tides or winds.

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OBJECTIVES

Computer modeling of highly complex, nonlinear, dynamical systems, such as that shown in Figure 1, brings together many scientific disciplines, including in our case, physical oceanography, meteorology, fluid dynamics, numerical methods, and computer science. Since, by definition, a model is a simplified portrayal of reality, successful model applications depend on how that simplification is realized. Thus, our primary research objective is to find the balance between the scale of physics to include in the model, the type of numerical algorithm, the amount of resolution, and the computational efficiency on parallel platforms in order to obtain accurate, robust, and timely simulations.

APPROACH

As presented in the original proposal, our specific approach to meeting the proposed objective is to study and advance four aspects of the current ADCIRC model: 1) compare several transport algorithms and program the most promising one into a transport code for prognostic baroclinic simulations; 2) understand the interplay between horizontal and vertical resolution for 3D simulations for both diagnostic and prognostic simulations; 3) define a criteria for switching between the finite element and discontinuous Galerkin solution algorithms; and 4) program the 3D version of the code to run in a distributed memory, parallel computing environment. In addition, we have undertaken two complementary tasks that were not part of the original scope of work: 5) look at alternative I/O paradigms to reduce output file sizes and speed up throughput; 6) develop a web-based grid library to archive the many computational grids that have been, and will be, developed by ADCIRC researchers. Key individuals and their roles are as follows (all are at the University of Oklahoma, unless noted otherwise): R. Kolar (PI), project oversight; J. Atkinson (post-doc), transport model development; K. Dresback (Ph.D. student), resolution studies and algorithms to compute the baroclinic pressure gradient; C. Szpilka (Ph.D. student) and C. Dawson (U. Texas), transport model development and discontinuous Galerkin/continuous Galerkin algorithm coupling; J. Dietrich (undergraduate researcher), numerical experiments; P. Quarles (M.S. student), grid data base; L. McSpadden (undergraduate researcher), visualization and I/O; J. Antonio, S. Dhall, S. Lakshmivarahan (Co-PI's), parallel programming.

WORK COMPLETED

Task 1 - Prognostic Baroclinic Simulations. These simulations require that the hydrodynamic model be dynamically linked to a transport model that has been fitted with an appropriate equation-of-state. It became evident during the early stages of this project that in order to test a variety of transport algorithms in a timely fashion, we needed to develop a 2D laterally averaged ("x-z") model, which takes about an order of magnitude less time to run than a comparable full 3D simulation. Moreover, analytical solutions exist to validate the algorithm in this reduced domain. Thus, the first year of the project was spent developing and verifying the x-z hydrodynamic model, which we have recently completed. Simultaneous with the x-z hydrodynamic code development, we spent time surveying the literature as to what other research groups have done with respect to the baroclinic transport. The results of that survey are guiding our development of the transport code. To serve as a baseline for comparison, we initially discretized the transport equation using a continuous Galerkin algorithm (same as that used for the hydrodynamics). However, literature and experience suggest that shock-

capturing algorithms (so-called TVD algorithms) may be a better fit for our intended applications, so we have also begun coding a transport code based on the discontinuous Galerkin method [2].

Task 2 - Resolution Studies. Since the prognostic code is still under development, these resolution studies have not begun. However, the current version of ADCIRC does have diagnostic capabilities, but they have not been rigorously tested on real basins. Consequently, as a first step toward "real" simulations, we tried simulating the Persian Gulf, which is known to have significant contributions to the flow field from the buoyancy terms (see Figure 1). The computational grid for this work is shown in Figure 2 below. To obtain meaningful results, three modifications were needed, as discussed in the Results section below.

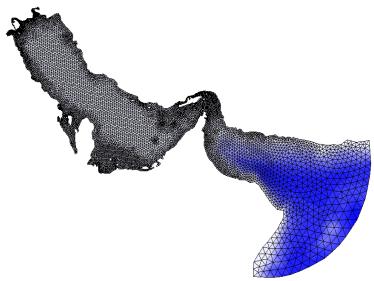


Figure 2. Computational mesh and bathymetry (darker blue for deeper bathymetry) for the Persian Gulf domain. Note that the use of triangular elements allows one to map irregular coastlines accurately and use graded meshes.

Task 3 - Algorithm Coupling. A truism in numerical methods is that there is no "best" algorithm, which also applies to the ADCIRC model. The Galerkin finite element, GWC (Generalized Wave Continuity) algorithm, which currently drives the ADCIRC model, is very efficient and accurate for slowly-evolving, deep water fields, but suffers from instabilities in highly advective regions. Thus, much effort has been spent over the last 10 years to search for a more stable algorithm; the discontinuous Galerkin (DG) method has emerged as the likely candidate. However, it is much less computational efficient than the GWC. So, an optimal solution for us appears to be to use the GWC in deep water and switch to the DG in shallow, near-shore regions [3]. Such a multi-algorithmic code raises new research issues, viz, how to couple the two algorithms and where in the domain to switch from one algorithm to the other. Our research group has developed a numerical analysis tool that quantifies the ability of an algorithm to propagate all possible wave frequencies, ranging from high frequency noise to long wave tidal motions [4]. We are applying this tool to first the DG algorithm, and then the coupled DG/GWC algorithm in order to verify that the coupling algorithm is indeed passing waves without distortion, and we are using the dispersion characteristics of the algorithm to develop criteria for switching between the two. Methods of coupling range from passing fluxes across interface boundaries to using an overlapping layer of elements at the interface.

Task 4 - Parallel Computing. Previous grants have supported efforts to parallelize the 2D version of ADCIRC using MPI and domain decomposition so that it runs on massively parallel clusters. During the past year, we have run extensive benchmarking tests on two different 16-processor platforms, and we have begun benchmarking efforts on a larger 256 node parallel cluster. 3D parallel coding and benchmarking has not progressed much during the past year.

Task 5 - File I/O. Full 3D simulations produce enormous volumes of output, which can be on the order of gigabytes. Consequently, an I/O strategy must be employed that is more efficient than the current ADCIRC standard, which is ASCII. Our team modified the ADCIRC code so that NetCDF (Network Common Data Form) can be used as an output option.

Task 6 - Grid Database. Currently, ADCIRC grids reside with the person(s) who developed the grid; when they are shared, little or no documentation is provided. During the past year, we have developed a web-based prototype for uploading, archiving, and retrieving ADCIRC finite element meshes. The archived files will contain all pertinent attributes for each grid, e.g., resolution, source of coastline and bathymetric data, software used to generate the mesh, meshing criteria, intended application for the grid, and security classification.

RESULTS

Task 1. An explicit CG transport requires such small time steps for stability, that it is not a viable algorithm for full 3D transport. Moreover, the algorithm is not stable at any time step for sharp front problems, such as a "dam break".

Task 2. Extensive testing, analysis, and debugging of ADCIRC led to the following modifications to the 3D diagnostic code: a better algorithm for computing baroclinic pressure gradients when neighbor nodes "run into the ground" (occurs in areas of steep bathymetric gradients); a different criteria for checking whether or not a vertical node is at or near the sea bed; a more robust procedure for using the OAX interpolating code [5, 6] to project the temperature and salinity field (data obtained from MODAS) onto the computational grid. Once these modifications were made, we were able to obtain realistic baroclinic simulations for the Persian Gulf, as shown in Figure 3 below.

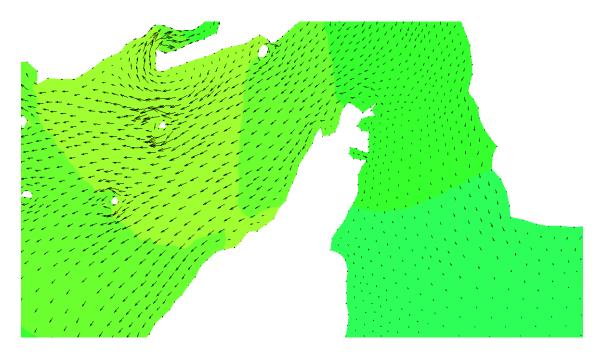


Figure 3. 3D diagnostic simulation results for the Persian Gulf using the density field shown in Figure 1 (expanded view of the center of the domain).

Task3. Work in this area is on-going, but two significant observations stand out. First, the aforementioned phase analysis tool has identified that partial coupling (e.g., applying DG to just the continuity equation) can introduce artificial oscillations in the solution unless slope limiters are applied, as shown in Figure 4 below. Recent applications have supported this theoretical result. Full DG/CG coupling through overlapping layers of elements appears to be promising (preserves amplitudes and phases across the interface), plus it follows the same paradigm that we use for domain decomposition [7].



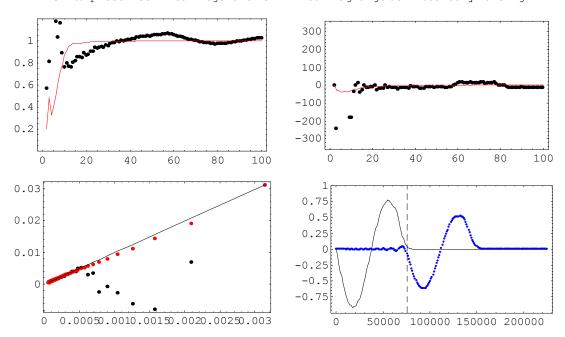


Figure 4. Phase analysis of partial DG/CG coupling: upper left and right frames show damping ratio and phase error vs. wavelength, respectively; lower left frame shows dispersion relation; lower right frame shows simulation result for 75dx wave. Note the oscillations in the solution, as indicated by the black dots, for high frequency waves.

Task 4. Benchmarking results indicate that the 2D code scales well on both 16 processor clusters, as shown in Figure 5, provided the problem size is large enough so that inter-processor communication does not dominate. Thus, the same paradigm (domain decomposition) will be used for the baroclinic 3D code.

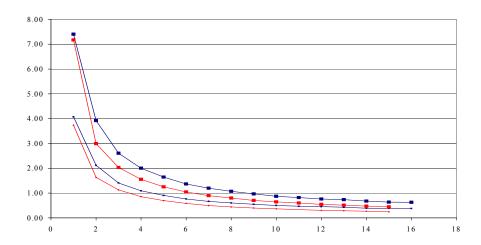


Figure 5. Benchmarking (wall-clock time vs. number of processors) of the 2D barotropic ADCIRC model on a 16-processor Sun Netra X1 cluster (navy line) and a 16-processor P3 Linux cluster (red line). Both show near theoretical speedup.

Task 5. In all test cases, the use of NetCDF reduced file size by 2/3 (as compared to ASCII), and, for I/O intensive simulations, the cpu time was cut by 1/2 [8].

Task 6. No significant results to report.

IMPACT/APPLICATIONS

Nothing to report at this time (first year of the project).

RELATED PROJECTS

With support from the US Army Corps of Engineers, Waterways Experiment Station, colleagues at the University of Notre Dame are working on a sediment transport algorithm that can be coupled to the ADCIRC model. This modification of the code is needed to be able to simulate the effects of coastal dredging and, thus, better manage coastal waterways. Sediment transport shares some of the same issues as salinity and temperature transport that we are working on; consequently, we are sharing research results, particularly since both groups are looking at similar transport algorithms (e.g., discontinuous Galerkin).

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